CHE221

SIMULATION LAB 1

-PRAGATI PATEL (230765) UG CHE

Aim of report:

Our assignment involves generating family of isotherm and adiabats for Peng Robinson Equation of State.We are also calculating PV work for isothermal and adiabatic process.

Introductory Theory:

Peng Robinson Equation of State Cubic equation of states (EOSs) can describe the behaviour of real gases. Consider a gas that is described by the Peng-Robinson cubic EOS:

$P = RT/(V - b) - \alpha a /(V (V + b) + b(V - b))$.

Area under PV graph is equal to work done.

An **isotherm** is a curve on a pressure-volume (P−VP-VP−V) diagram that represents the relationship between the pressure and volume of a gas at a constant temperature.

An **adiabatic curve** represents the relationship between two thermodynamic variables (like pressure, temperature, or volume) when the process occurs without any heat exchange.

Constants used:

a= 0.45724*R^2*Tc^2/Pc

b= 0.07780*R*Tc/Pc

$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega 2$.

alpha=(1+k(1-(T/Tc)^0.5))^2

Cv(T) = 20 + 0.01*T + 10−5T^ 2

For this problem, assume R = 8.314 J/(mol · K), Tc = 304.2 K, Pc = 7.38 × 106 Pa, and ω = 0.225

Methodology:

1)Generate a set of **isotherms**, i.e., pressure vs. volume curves at constant temperatures, for a real gas using the Peng-Robinson equation of state.

2)Generate **adiabatic curves** (T-V curves) where temperature T changes as volume V varies, under adiabatic conditions.

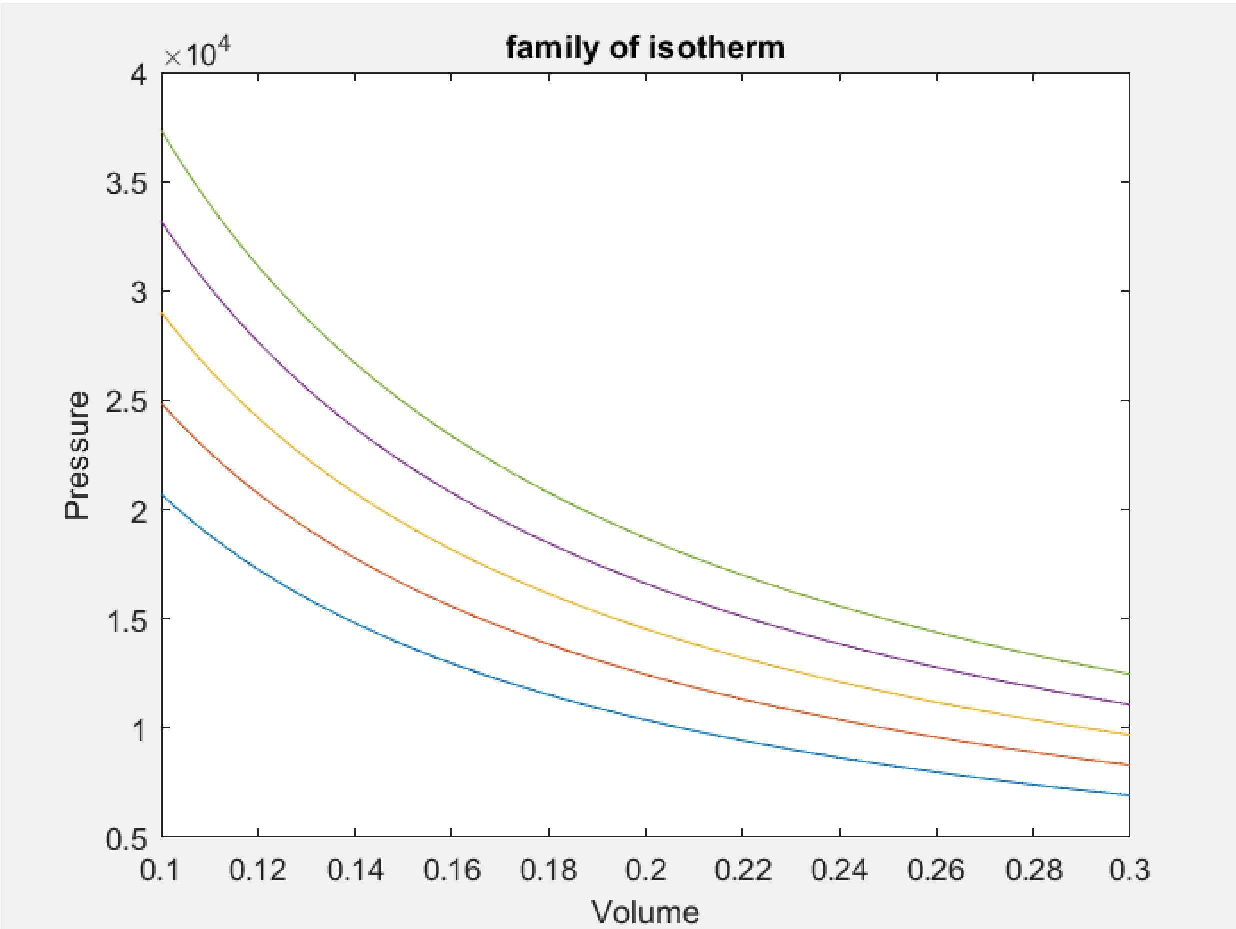
3)Generate a Family of Adiabats (P-V Curves) for the Peng-Robinson EOS.

4)Calculate the PV Work for an Adiabatic Process.Numerically integrate the pressure over the volume range (0.1 m^3 to 0.3 m^3) using a numerical integration method such as the trapezoidal rule (`trapz` function in MATLAB).

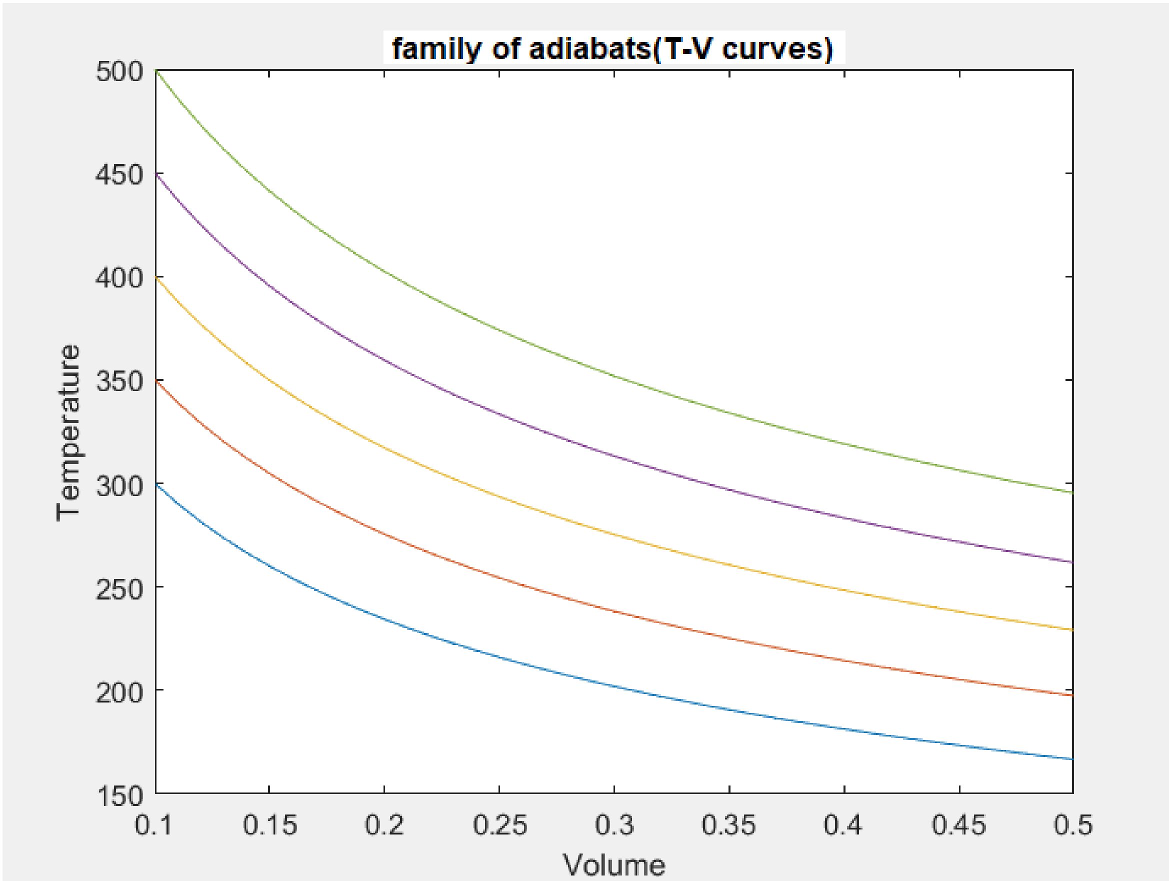
Thus,work done for adiabatic process=2.2628e+03J

5)Calculate the PV Work for an Isothermal Process.Use trapz function.

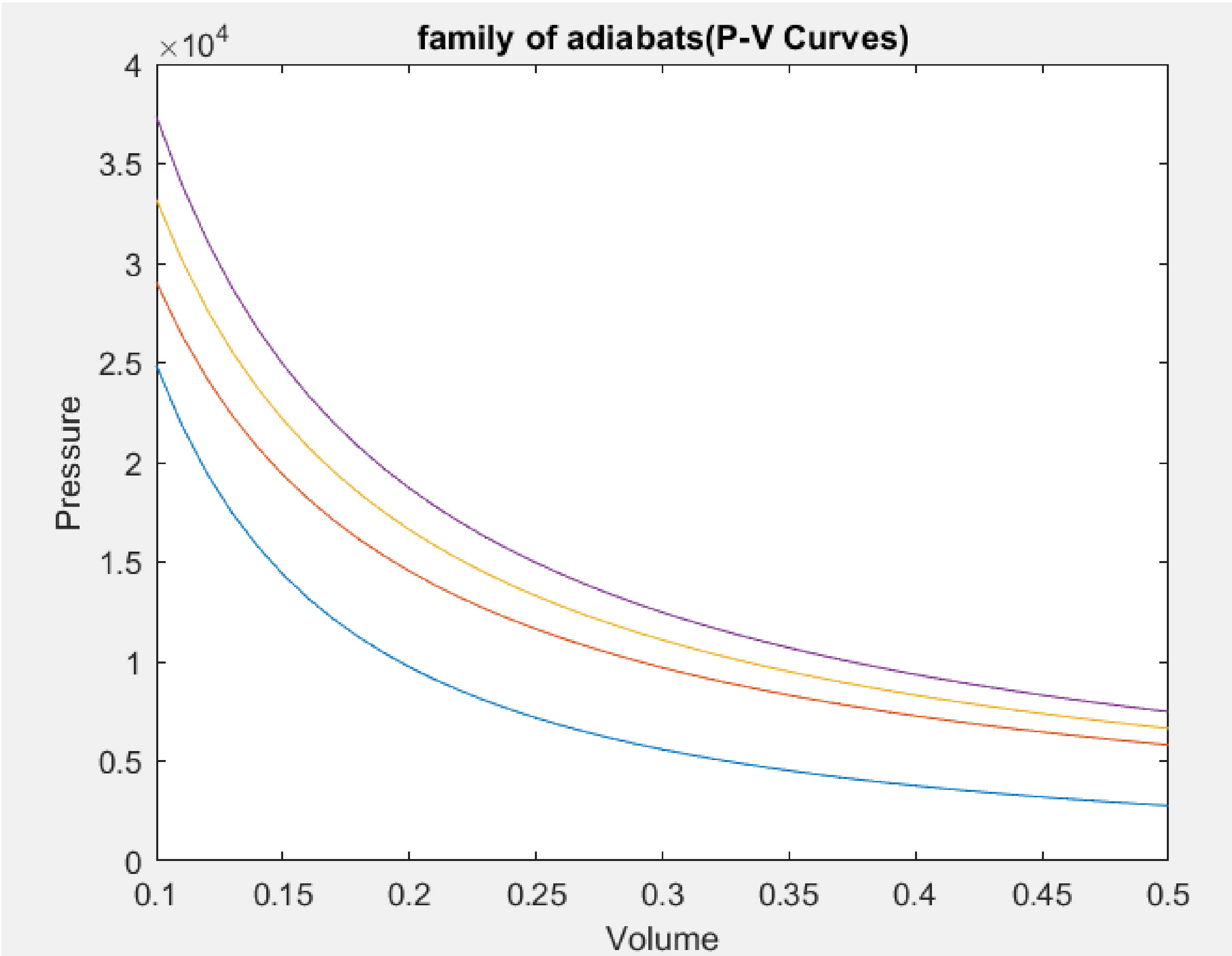
Thus,work done for isothermal process=2.7358e+03J

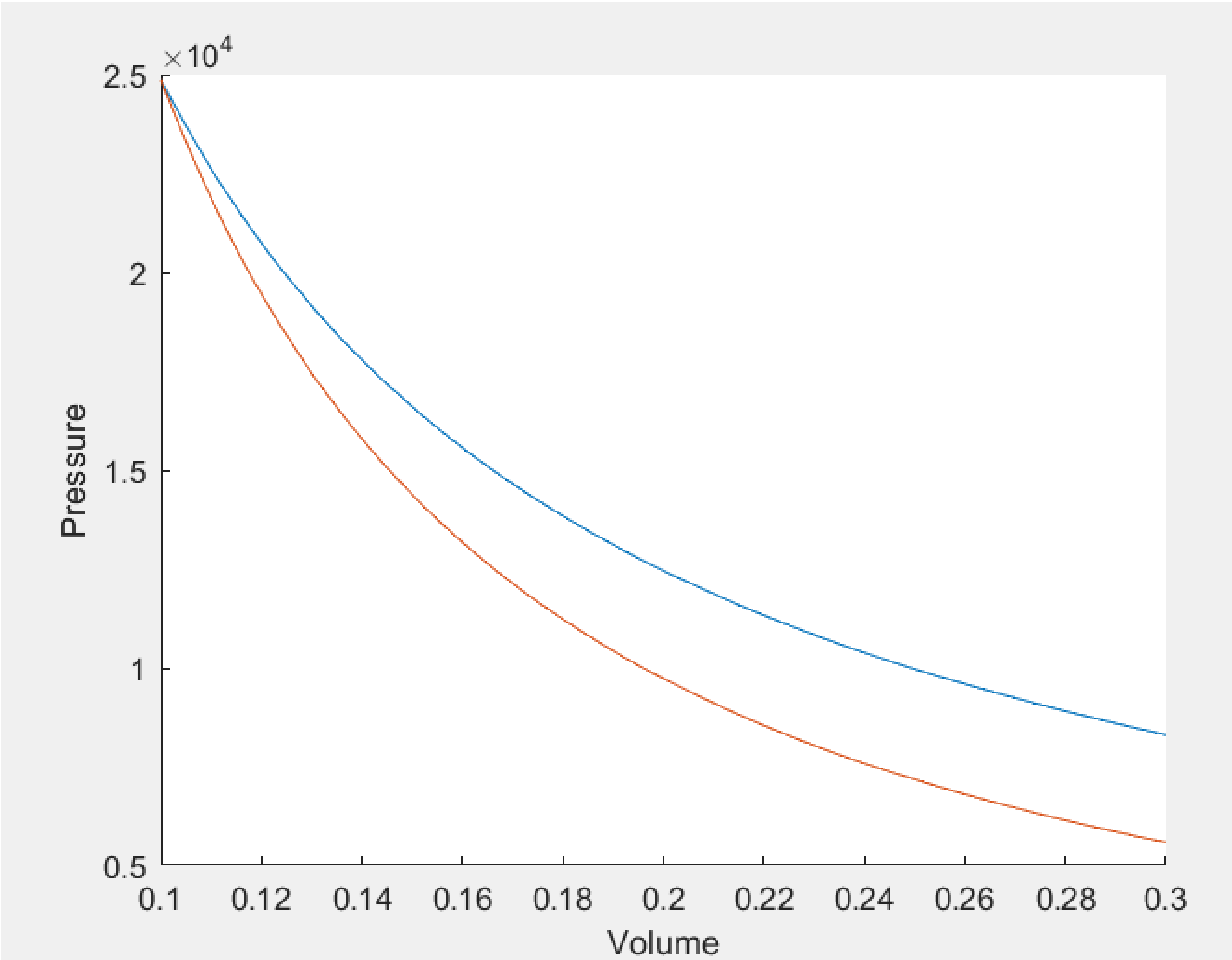


family of isotherm
×10^4
4
3.5
3
2.5
2
1.5
1
0.5
Pressure
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
0.28
0.3
Volume



family of adiabats(T-V curves)
Temperature
500
450
400
350
300
250
200
150
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
Volume


family of adiabats(P-V Curves)
×10^4
4
3.5
3
2.5
2
1.5
1
0.5
0
Pressure
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
Volume



Appendix:

```
clear
clc
w=0.225;
P_c=7.38*1e6;
T_c=304.2;
R=8.314;
k=0.37464+1.54226*w-0.26992*(w^2);
a=(0.45724*(R^2)*(T_c^2))/P_c;
b=(0.07780*R*T_c)/P_c;
alpha = @(T) (1+k.*(1-(T./T_c).^1/2)).^2;
P = @(V,T) (R.*T)./(V-b)-(alpha(T).*a)./(V.*(V+b)+b.*(V-b));
V = linspace(0.1,0.3,100);
```

```
%isothermal curve
figure
plot(V,P(V,250))
hold on
plot(V,P(V,300))
plot(V,P(V,350))
plot(V,P(V,400))
plot(V,P(V,450))
hold off
xlabel('Volume')
ylabel('Pressure')
Cv = @(T) 20+0.01.*T+(1e-5).*(T).^2;
d_alpha_dT = @(T) -k./sqrt(T*T_c).*(1+k-k.*sqrt(T/T_c));
dP_dT= @(V,T) (R)./(V-b)-(d_alpha_dT(T).*a)./(V.*(V+b)+b.*(V-b));
%adiabatic ode (T-V curve)
dT_dV = @(V,T) ((-T).*(dP_dT(V,T)))./Cv(T);
V_span=[0.1,0.5];
figure
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,300);
plot(V_adiab,T_adaib)
hold on
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,350);
plot(V_adiab,T_adaib)
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,400);
plot(V_adiab,T_adaib)
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,450);
plot(V_adiab,T_adaib)
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,500);
plot(V_adiab,T_adaib)
hold off
xlabel('Volume')
ylabel('Temperature')
%adiabatic ode (P-V curve)
figure
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,300);
plot(V_adiab,P(V_adiab,T_adaib))
hold on
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,350);
plot(V_adiab,P(V_adiab,350))
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,400);
plot(V_adiab,P(V_adiab,400))
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,450);
plot(V_adiab,P(V_adiab,450))
hold off
xlabel('Volume')
ylabel('Pressure')
%P-V work for adiabatic process
V_span=linspace(0.1,0.3,100);
[V_adiab,T_adaib]=ode45(@(V,T) dT_dV(V,T),V_span,300);
```

```
P0=P(V_adiab,T_adaib);
A1=trapz(V_span,P0)
%P-V work for isothermal process
V1=linspace(0.1,0.3,100);
P1=P(V1,300);
A2=trapz(V1,P1)
%PLOT FOR ISOTHERMAL AND ADIABATIC PROCESS
V3 = linspace(0.1,0.3,100);
figure
hold on
plot(V3,P(V3,300));
[V_adiab,T_adaib]=ode45(@(V3,T) dT_dV(V3,T),V3,300);
plot(V_adiab,P(V_adiab,T_adaib))
hold off
xlabel('Volume')
ylabel('Pressure')
```

Conclusion

The Peng-Robinson EOS successfully captured the behavior of real gases under isothermal and adiabatic conditions.
Work done in the isothermal process was larger than that in the adiabatic process for the given conditions